RANDOM FIELD MODELS FOR RELAXOR FERROELECTRIC BEHAVIOR

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Heat bath Monte Carlo simulations have been used to study a four-state clock model with a type of random field on simple cubic lattices. The model has the standard nonrandom two-spin exchange term with coupling energy J and a random field which consists of adding an energy D to one of the four spin states, chosen randomly at each site. This Ashkin-Teller-like model does not separate; the two random-field Ising model components are coupled. When $D/J = 3$, the ground states of the model remain fully aligned. When $D/J \geq 4$, a different type of ground state is found, in which the occupation of two of the four spin states is close to 50%, and the other two are nearly absent. This means that one of the Ising components is almost completely ordered, while the other one has only short-range correlations. A large peak in the structure factor $S(k)$ appears at small k for temperatures well above the transition to long-range order, and the appearance of this peak is associated with slow, "glassy" dynamics. The phase transition into the state where one Ising component is long-range ordered appears to be first order, but the latent heat is very small.

I. INTRODUCTION

Shortly after the seminal work of Imry and Ma[1] on the effects of random fields in ferromagnets, it was pointed out by Halperin and Varma[2] that similar ideas could be used to understand the effects of atomic disorder in perovskite ferroelectrics. Halperin and Varma showed that atomic disorder which coupled linearly to the ferroelectric order parameter behaved in an equivalent fashion to the random field in a ferromagnet, and thus could cause the ferroelectric phase transition to become smeared. They seem to have been unaware, however, that ferroelectrics displaying such smeared transitions had been discovered long before.[3] These materials, now called relaxor ferroelectrics, were originally referred to as ferroelectrics with diffuse phase transitions. The random-field ideas of Halperin and Varma did not immediately become popular in the field. In the 1984 review of Isupov[4] the diffuse phase transitions were modeled using only random-bond disorder. However, by the early 1990's it was generally recognized that random-bond disorder was not enough to explain all of the observed effects, and models including both random bonds and random fields became widely used.[5,6,7,8] Until now it has been assumed[7,8] that in the presence of a strong cubic crystal-field anisotropy one could treat the different Ising components independently. In this work we will show that for a certain type of random field new phenomena occur which cannot be understood without including coupling between the components.

The identification of relaxor ferroelectrics as a broad class of materials in which electric dipoles behave in a manner analogous in many respects to the magnetic dipoles in spin-glasses was made forcefully by Burns and Dacol,[9] who generalized and extended ideas of Courtens.[10] It is essential, however, to note that, as shown by Halperin and Varma,[2] in the case of electric dipoles it is almost inevitable that the disorder which is

an essential feature of these materials will produce random fields. The presence of these random fields limits the development of long-range spin-glass order in three dimensions.[11] Therefore, it is not expected that the glassy behavior which is seen in the disordered electric dipole materials represents a true phase transition into a state with long-range spin-glass-type order.

We would like to study the development of spatial correlations among the electric dipoles. In order to do this, we will work with a model which does not retain all of the atomic details. In the model studied here, we crudely represent each perovskite unit cell by only one dynamical variable. We will refer to this variable as a spin, although it actually represents atomic displacements in the unit cell. The model includes a cubic crystal anisotropy, a nearest-neighbor two-spin interaction, and a random field.

As discussed by Pirc and Blinc,[8] if we assume that the cubic crystal anisotropy is so strong that each spin points along one of the [111] directions and the random field is represented by a simple vector coupling linearly to the spin, then the different components of the spin act independently.[12] Thus the model reduces to a set of decoupled random-field Ising models. We may also include randomness in the bonds. (To perform this decoupling on Eq. (1), we use a coordinate system rotated by 45°.) This model has been studied in detail over a number of years. It is believed to be generally well-understood, although there remains some controversy about the values of the critical exponents.[13,14]

Similar models have been studied in which the spin components do not act independently. Then the behavior does not reduce to that of an Ising model. For example, there are the three-state Potts model with a random field,[15] and the four-state Potts model with a random field,[16] which are still qualitatively similar to the random-field Ising model. When the random field becomes strong enough, the ground state of the system breaks up into

Imry-Ma domains, and the long-range order is destroyed.

There is also the cubic model with random anisotropy,[17] which, when the randomness is strong, shows a new type of domain phase with long-range order. This phase may be thought of as one in which each of the spin components orders independently, but different parts of the lattice are dominated by different components. Thus, in this phase, there is a network of 90° domain walls embedded in the ordered phase. A somewhat similar domain state was found by Kartha, Castan, Krumhansl and Sethna[18] in a model of shape-memory alloys.

The existence of such a domain state with long-range order has been proposed[19,20] as the explanation of relaxor ferroelectric behavior. Further, Egami[21] has emphasized that the network of 90° domain walls is probably an essential element leading to the large piezoelectric response of relaxor ferroelectrics. Therefore, we would like to study a random-field model which has such a phase.

II.   THE MODEL

The simplest model which has the desired properties is a four-state vector Potts model (four-state clock model) with a random Potts field, on a simple cubic lattice. The Hamiltonian of this model is

$$H = -J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + h_r \sum_i \delta_{\mathbf{S}_i, \mathbf{n}_i} \,. \qquad (1)$$

Each spin $\mathbf{S}_i$ is a dynamical variable which has four allowed states: (1,0), (0,1), (-1,0) and (0,-1). Each $\mathbf{n}_i$ is an independent quenched random variable which assumes one of these four allowed states with equal probability. The $\langle ij \rangle$ indicates a sum over nearest neighbors of a simple cubic lattice. The extension to three-component spins is conceptually straightforward, but will not be discussed in detail here.

The sign of h_r is chosen so that for large positive values the probability of spin $\mathbf{S}_i$ in state $\mathbf{n}_i$ is strongly suppressed. Density-functional calculations for a typical relaxor ferroelectric alloy[22] have shown that the most significant interactions created by the alloy disorder are repulsive and short-ranged. Thus we believe that this is a reasonable first approximation to the interactions produced by the disorder.

When h_r is negative, the random Potts field favors one state on each site, just as a vector field would. In that case there is no qualitative difference between the random Potts field and the random vector field.[23,24] Thus we will not present any calculations for negative h_r here.

When h_r is large and positive, we can approximate the random field term as a projection operator which forbids $\mathbf{S}_i$ from occupying the state $\mathbf{n}_i$. Then within mean-field theory it becomes simple to calculate the approximate ground states. There are eight of these mean-field ground states. For example, in one such ground state 75% of the spins are in state (1,0), and the other 25% of the spins,

which are prevented from being in this spin state by their local $\mathbf{n}_i$ are in state (0,-1). The energy of this state for a simple cubic lattice is easily calculated to be $-1.875 \, J$ per spin. Additional details of the mean-field theory are discussed in the Appendix.

As we will see, the energies of the ground states found by computer calculation are less than $-2 \, J$, and they differ qualitatively from the mean-field ground states. The problem with the mean-field ground states is easy to understand. If we consider the above example, on a simple cubic lattice the 25% of spins in the state (0,-1) are broken up into finite clusters. If we move all of the spins in such a finite cluster into the state (0,1), the total energy does not change. One might expect, therefore, that for large h_r, the long-range order in the ground state would still be along one of the four [1,0] directions, since the 25% of the spins in the finite clusters should not be able to exhibit long-range order.

However, a true ground state on the simple cubic lattice actually has a very different structure. It turns out to be possible to find states with, for example, 50% of the spins in state (1,0) and 50% of the spins in state (0,-1) which have a much lower energy than the mean-field ground states. As we will show, to find states which look like the true ground states for large h_r within mean-field theory, we need to add another term to Eq. (1).

The author finds it helpful to compare the model studied here to the results for the three dimensional Ashkin-Teller model,[25] whose Hamiltonian is

$$H_{AT} = -J \sum_{\langle ij \rangle} (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j) - 2J_4 \sum_{\langle ij \rangle} (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)(\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j) \,, \qquad (2)$$

where $\boldsymbol{\sigma} = \pm\frac{1}{2}(1,1)$ and $\boldsymbol{\tau} = \pm\frac{1}{2}(1,-1)$ are Ising variables. (Note that our notation and normalization differ from those of Ditzian et al.[25])

Each of the three linearly independent components of a random field of a four-state model can now be identified with one of the terms of Eq. (2), and thus one of the mean-field order parameters. Expressing the random-field term using the $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$ variables, and adding it to Eq. (2), we get

$$H_{RFAT} = H_{AT} + (h_r/4) \sum_i [1 + 2(\boldsymbol{\sigma}_i \cdot \mathbf{n}_i) + 2(\boldsymbol{\tau}_i \cdot \mathbf{n}_i) + 4\eta(\boldsymbol{\sigma}_i \cdot \mathbf{n}_i)(\boldsymbol{\tau}_i \cdot \mathbf{n}_i)] \,. \qquad (3)$$

If we set $\eta = 1$ and $J_4 = 0$, then Eq. (3) becomes just Eq. (1) expressed in the coordinate system defined by $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$. If we then set $\eta = 0$, the random Potts field term is replaced by the usual random vector field term.

In a real alloy we would not expect that exactly one of the local states was blocked on each site. Instead, we would expect to find a random distribution, with some sites having no blocked states, some with one blocked state, etc. It would be straightforward to generalize the random field term to allow this, by letting η in Eq. (3) become a function of i. For example, we could use a probability distribution for η_i which had weight at ± 1. Such a generalization is likely to be useful in modeling

the properties of specific alloy systems. However, a more general model has more parameters. Exploring its entire parameter space would be tedious, and seems premature at this time.

III. PHASE DIAGRAM

If h_r/J is chosen to be an integer, then the energy of any state is an integer multiple of J. Then it becomes straightforward to design a heat bath Monte Carlo computer program to study Eq. (1) which uses integer arithmetic for the energies, and a look-up table to calculate Boltzmann factors. This substantially improves the performance of the computer program, and was used for all the calculations reported here. (If desired, one could do almost as well for half-integer values of h_r/J.) Lattices with periodic boundary conditions were used throughout. Two different linear congruential random number generators were used: one to choose the random $\mathbf{n}_i$ and one to choose the Boltzmann factors for the Monte Carlo spin flips.

A series of $L \times L \times L$ samples of various lattice sizes and values of h_r was studied to map out the phase diagram, which is shown in Fig. 1. For $h_r/J \leq 3$ the behavior of the random Potts field model remains generally similar to the behavior of the random vector field model. At low temperature the system develops long-range order, with the order parameter aligned along one of the spin-coordinate axes. It is not required, however, that the critical exponents for the phase transition here will be those of the random-field Ising model, as happens for the vector random-field case.

The $\langle \boldsymbol{\sigma} \rangle$ phase found by Ditzian, Banavar, Grest and Kadanoff[25] has many of the features of the domain FE phase which we find in our model for large h_r and low T. The $\langle \boldsymbol{\sigma} \rangle$ phase of Eq. 2 only occurs for $J_4 < 0$. This indicates that one of the effects of the random Potts field in Eq. (1) is to generate a negative effective value of the J_4 coupling. This effect was also seen in the random-anisotropy cubic model.[17] It is the random-anisotropy part (the η term of Eq. (3)) which generates the J_4 effective coupling under rescaling, and prevents the decoupling of Eq. (1) into two Ising models. If we want to study a mean-field theory for Eq. (1) we should include a J_4 term, thus arriving at Eq. (3). The effective value of J_4 will depend on h_r. In this way we can obtain a mean-field theory which reproduces the phase diagram of Fig. 1.

A necessary condition for the existence of stable long-range [1,1] domain FE order is that there be infinite connected clusters of both of the two dominant spin states. Since it becomes impossible to fulfill this condition when the amount of long-range order is small, the transition from the domain FE phase to the paraelectric phase must be first order. This, however, is specific to our model with only first neighbor interactions on the simple cubic lattice. It is possible that this phase transition could become

continuous if, for example, second neighbor exchange is included in the Hamiltonian.

As discussed by Ditzian et $al.$[25], even in the absence of randomness the details of what happens as we move from the $\langle \boldsymbol{\sigma} \rangle$ phase to the Baxter phase are not clear. There may be a small area in the region of the [1,0] FE to [1,1] domain FE phase boundary in which an intermediate phase is stable. This would be similar to the intermediate phase which has recently been found experimentally.[26] We have indicated the uncertainty about what is going on in this region of the phase diagram by the question mark in Fig. 1. A generalization of the $\langle \boldsymbol{\sigma} \rangle$ phase also exists for the three-component Ashkin-Teller model in three dimensions.[27]

The dotted line in Fig. 1 represents the approximate location of the onset of thermal hysteresis. Above the dotted line, the system will quickly relax to a state which is independent of initial conditions, but below this line the system retains a memory of initial conditions for a long time. This line does not represent any true thermodynamic singularity. Its precise location depends somewhat on the size of L and the length of the Monte Carlo runs. Thus the dotted line should be identified as the glass temperature, T_g. For small values of L the system can develop order on the scale of L above T_g. For $L = 64$ and $h_r \geq 3$ it is not possible to find the ground states in a reasonable time by cooling the system from high temperature.

IV. SPECIFIC HEAT

In Fig. 2 we display the specific heat for Eq. (1) using four different values of h_r. These curves were calculated by numerically differentiating and averaging Monte Carlo data for the energy of runs for four $L = 64$ lattices for each value of h_r, starting at high temperature and cooling slowly. For each run, the temperature was changed in steps of $0.05J$. 40,960 Monte Carlo passes through the lattice were performed at each value of T, with data being collected after each 20 passes. The first 248 data points at each temperature were discarded, and the remaining 1,800 data points were averaged. A similar procedure was used for heating runs.

Note that for $h_r = 0$ (not displayed), the specific heat for Eq. (1) reduces to a that of an ordinary Ising model on the simple cubic lattice, with $T_c/J = 2.256$. This model has a very sharp singularity at T_c, whose height diverges to infinity with L. We see in Fig. 2 that as h_r increases, the peak in the specific heat broadens and shifts to lower energy, with approximately half of the change occurring by $h_r = 3$. By comparing with Fig. 1, it is seen that for $h_r > 0$ the peak in the specific heat is centered above the region of glassy behavior. The average heights and widths of the peaks shown in Fig. 2 are essentially the same for $L = 32$ (not shown) as for $L = 64$. As one would expect, there is more variation from sample to sample for the smaller lattices.

In Fig. 3 we compare data from the cooling runs with $h_r = 6$ with heating runs on the same lattices. The initial condition for each heating run was a state with long-range order. The temperature at which the long-range order collapses is identified as T_g. We see that below T_g there is a region of T where the specific heat is slightly higher for the cold-start sample. The crossing of the two curves near $T/J = 1.2$ gives us a crude estimate for the ordering temperature T_c.

It is often possible to estimate T_c for a first-order phase transition with high precision. In order to do this with a computer simulation, however, it is necessary to run the simulation close to T_c, with L larger than the correlation length, for a time which is long enough so that the sample can spontaneously order and disorder several times. We are far from being able to satisfy that condition here, due to the glassy dynamics for $T < T_g$.

The integrated area between the cooling curve data and the heating curve data gives us an estimate of the value of the latent heat at T_c. We can also look directly at the difference in energy between the heating run and the cooling run at $T = 1.2 \ J$. Thus we find that the latent is about $0.01 \ J$. The fact that the slope of the heating curve is so similar to that of the cooling curve and the latent heat at T_c is so small indicates that there is very little difference in the local structure of this model between the ordered states of the [1,1] domain ferroelectric phase and the metastable states which are found by slow cooling. A small latent heat is a natural consequence of a large (but finite) correlation length at T_c.

V.   CORRELATION FUNCTIONS

In order to obtain information about the two-spin correlations, we calculate the angle-averaged structure factor $S(k)$. In Fig. 4 we display a log-log plot of $S(k)$, obtained by averaging over the data from the cooling runs for the $L = 64$ lattices, as a function of T/J. We see that for all these values of $h_r \geq 3$, the qualitative behavior of a sample cooled from high T without any external ordering field is the same. As we lower T, the peak near $k = 0$ first grows and then saturates. The rate of growth of this peak is maximal at the temperature where the specific heat has its maximum. As h_r decreases, the height of the peak and the value of the correlation length increase. For $h_r = 3$, the correlation length at low T becomes larger than our sample size. However, these zero-field-cooled samples never show true long-range order. With true long-range order, the size of the small-k peak would decrease as T decreases below T_c, because the intensity in the long-range-order δ-function will not appear on the log-log plot.

In Fig. 5 we show data for $S(k)$ from the heating runs, where the samples begin in an ordered state. Under these conditions, the size of the small-k peak continues to grow as T is increased above T_c, until T reaches T_g and the sample can equilibrate. In Fig. 5(c) we show data from

runs which are ten times longer than the standard runs. The $h_r = 4$ samples are able to equilibrate at $T/J = 1.7$ during the long run (*i.e.* they become indistinguishable from the data from the corresponding cooling run), but the changes at $T/J = 1.5$ are small. By $T/J = 1.4$ increasing the length of the run by a factor of ten has a negligible effect on the observed state of the sample.

VI.   GROUND STATES

Somewhat surprisingly, it turned out to be possible to find approximate ground states of the $h_r = \infty$ samples by a simulated annealing procedure. In Fig. 6 we show $S(k)$ for the approximate ground states of the $L = 64$ lattices with $h_r = \infty$, averaging over each of the four [1,1] directions for each of the four samples. The data shown in the figure are fit quite well with by a Lorentzian line shape, with a correlation length of about 10 lattice units. This diffuse-scattering part of $S(k)$ contains about 54% of the spectral weight. The other 46% of the weight is in the δ-function at $k = 0$, which is due to the long-range [1,1] order.

What this means in detail is that for large h_r a ground state contains approximately 49% each of the two majority spin states, and about 1% each of the two minority states. The energy per spin of the lowest ground states found for each sample was about $-2.010 \ J$, with the energies of the "ground states" of the same sample in the other three [1,1] directions lying typically about $0.003 \ J$ higher. Since $L = 64$ is large compared to a correlation length of 10, this result for the ground state energy should represent the large L limit, while the differences in energies between alternate ground state directions of the same sample should scale like $1/L^{3/2}$. Note that these actual ground state energies are substantially below the energy of the simple mean-field ground state of the $h_r = \infty$ model.

For $L = 64$ and $h_r = \infty$ the energy of a zero-field-cooled state at $T = 0$, which has no long-range order, is only about $0.01 \ J$ higher than the energy of a true ground state. Thus for lattices smaller than about $L = 32$ the energy differences between the ground states of different [1,1] directions become larger than the energy difference between a zero-field-cooled state and a true ground state. Under these conditions the zero-field-cooled sample is able to reach a long-range-ordered state. The zero-field-cooled $L = 64$ samples can be decomposed into domains of different [1,1] ground states, with 90° walls between the domains.

The probabilities of having effective fields of magnitude 6, 5, ... and 0 in a ground state, averaged over the four ground states for each of these $L = 64 \ h_r = \infty$ samples are 0.1121, 0.2780, 0.3148, 0.1685, 0.0751, 0.0383, and 0.0131, respectively. Thus, in a ground state only about one spin in nine is surrounded by fully aligned nearest neighbors. More than 1% of the spins are in zero effective field.

Some of the spins can flip freely between two positions in a ground state with no cost in energy. Since the spins in this model are discrete and two-dimensional, being in zero effective field is not a necessary condition for a spin to be "free" in this way. The bulk of these free spins are flipping between the two majority spin states for that particular ground state. It is easy to find that the fraction of free spins in a particular ground state is about 6.5%. However, a spin which is not free in one ground state may become free by the flipping of other free spins. The fraction of spins which can become free by the flipping of other free spins, one at a time, is 11.9%. Since 0.119 is much less than the critical concentration for uncorrelated site percolation on a simple cubic lattice, it is not surprising that a set of free spins defined in this way consists of small isolated clusters.

The probability that a free spin may occupy all three of its allowed spin states with no energy cost is negligible to this level of accuracy. Thus a lower bound on the ground state entropy per spin for large h_r is 0.065 $ln(2)$, and 0.119 $ln(2)$ is an upper bound. Calculating the ground state entropy of this model is a complex problem, because it requires finding all of the ground states.

Thus each of the four "[1,1] ground states" of a sample is actually a cluster of ground states in the phase space of the model. The simulated annealing procedure works because, if we use one of the simple mean-field ground states, which has 75% of the spins in one spin state and 25% of the spins in a second spin state, as an initial condition, the direction of the order parameter will rapidly relax to the closest of the [1,1] energy minima, even at temperatures well below T_c. The fact that this is possible is partly due to the large number of spin rearrangements which can be made with no energy cost. This prevents the system from being easily trapped in a metastable minimum of the free energy which is close to the initial mean-field ground state.

Although a ground state energy of $-2.01\ J$ means that about 33% of nearest neighbor spin pairs are oriented at $90°$ from one another, the fraction of nearest neighbor spin pairs which are pointing in opposite directions in one of these ground states is only 0.00011. The small number of spins in the minority states exist in compact blobs whose diameter is approximately the correlation length of 10 lattice units.

For $h_r/J = 3$, every sample studied had four ground states, each one fully aligned along one of the four [1,0] spin states. There is an exponentially small probability of having an unusual local configuration of the $\mathbf{n}_i$ which would misalign a small cluster of spins in a ground state, but this was never observed. Thus, ignoring the statistical fluctuations in the sample average of $\mathbf{n}_i$, the ground state energy in the [1,0] ferroelectric phase is found to be $E_0 = -3\ J + 0.25\ h_r$. The value of E_0 for any value of h_r cannot be greater than $-2.01\ J$, its value for $h_r = \infty$. From this we expect that the boundary between the [1,0] phase and the [1,1] domain phase should be at h_r/J slightly less than 4, as observed.

VII. DISCUSSION

In the past, various kinds of evidence have been presented to argue that relaxor ferroelectrics represent a distinct class of materials, and are not merely the inevitable consequence of adding some alloy disorder to any ferroelectric. De Yoreo, Pohl and Burns[28] studied the low-temperature properties of a variety of ferroelectric alloys, and found that they could be separated into two classes. Relaxor ferroelectrics showed glassy low temperature behavior and normal ferroelectrics did not, even when the normal ferroelectrics were random alloys. Recently, Viehland *et al.*[29,30,31] have argued that in some materials they find a well-defined transition between a normal ferroelectric phase and a relaxor ferroelectric phase. It would be remarkable if the low temperature thermal properties of such a crystal could be switched from glassy behavior to crystalline behavior by poling the sample. To the author's knowledge, this experiment has not yet been tried.

For the two-spin exchange interaction of Eq. (1), a $180°$ domain wall has twice the energy of a $90°$ domain wall. As a result of this, $180°$ domain walls become rare at low temperature in this model. As pointed out by Bürgel, Kleemann and Bianchi,[20] ferroelastic interactions raise the energy of $90°$ walls, but do not have much effect on the energy of $180°$ walls.

To incorporate this effect into our model, we would add a biquadratic term to Eq. (1) of the form $-K(\mathbf{S}_i \cdot \mathbf{S}_j)^2$. When K/J becomes large, the structure of the domain state will change,[20] because $180°$ domain walls now have a lower energy than $90°$ domain walls. It is difficult to study this Bürgel, Kleemann, Bianchi domain state with computer simulations if the size of a ferroelastic domain is large. A sample which is the size of a single ferroelastic domain (or smaller) will behave essentially as a random-field Ising model.

VIII. CONCLUSION

In this work we have used Monte Carlo computer simulations to study a simple model of a ferroelectric alloy. In this model, the alloy disorder causes some of the positions of the polarizable ions to be strongly disfavored. We have found that this model displays a type of ferroelectric domain phase which does not exist in the model of Pirc and Blinc.[8] This phase may be thought of as resulting from the addition of a random field to the $\langle \boldsymbol{\sigma} \rangle$ phase[25] of an Ashkin-Teller model. It seems likely that this model, and some natural generalizations of it, will help in the understanding of relaxor ferroelectric behavior.

APPENDIX: MEAN FIELD THEORY

The presence of the random field greatly complicates the mean-field theory for Eq. (1). It is necessary to distin-

guish the four classes of spins corresponding to the four different allowed values of $\mathbf{n}$. Label the four directions (1,0), (0,1), (-1,0) and (0,-1) as direction 1, 2, 3 and 4, respectively. Define $p_{\mu\nu}$ to be the probability that a spin of class μ points in the ν direction. Then $\sum_\nu p_{\mu\nu} = 1$ for any μ. But, in the general case, we have to deal with twelve independent variables in the mean-field theory. If we take the limit that h_r becomes infinite, there are only eight independent variables, because we can then set $p_{\mu\nu}$ to 0 when $\mu = \nu$.

Let z be the number of neighbors of any spin. Then the mean-field expression for the energy per spin is

$$E = -(zJ/32) \sum_{\mu,\nu,\mu',\nu'} p_{\mu\nu} p_{\mu'\nu'} \cos(\pi(\nu - \nu')/2) . \quad \text{(A.1)}$$

In addition to the usual factor of 1/2 to avoid double-counting, there is factor of 1/16 arising from the assumption that each value of μ (*i.e.* each $\mathbf{n}$) is equally weighted.

The entropy per spin is

$$S = -1/4 \sum_{\mu,\nu} p_{\mu\nu} \ln(p_{\mu\nu}) , \quad \text{(A.2)}$$

and the free energy is, as usual, $F = E - TS$. Then solving the mean-field theory requires finding the minimum of $F(T)$ in the phase space of the $p_{\mu\nu}$.

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FIG. 1: Phase diagram of the random Potts field model on simple cubic lattices, showing the paraelectric (PE), ferro-electric (FE), and domain FE phases. The solid lines indicate first-order transitions, and the dashed line indicate the approximate onset of glassy dynamics in the PE phase. The question mark is discussed in the text.

FIG. 2: Specific heat vs. temperature for the random Potts field model on $64 \times 64 \times 64$ simple cubic lattices, for various values of h_r. Data from zero-field-cooled runs, averaging data from four samples.

FIG. 3: Specific heat vs. temperature for the random Potts field model on $64 \times 64 \times 64$ simple cubic lattices, for $h_r = 6$, averaging data from four samples. The solid line shows zero-field-cooled data using a random initial condition, and the dashed line shows zero-field-heated data using an ordered initial condition.

FIG. 4: Angle-averaged magnetic structure factor at a sequence of temperatures for the random Potts field model on $64 \times 64 \times 64$ simple cubic lattices, log-log plot. The points show averaged data from four samples, using zero-field-cooling and a random initial condition. (a) $h_r = \infty$; (b) $h_r = 6$; (c) $h_r = 4$; (d) $h_r = 3$.

FIG. 5: Angle-averaged magnetic structure factor at a sequence of temperatures for the random Potts field model on $64 \times 64 \times 64$ simple cubic lattices, log-log plot. The points show averaged data from four samples, using zero-field-heating and an ordered initial condition. (a) $h_r = 6$; (b) $h_r = 4$; (c) $h_r = 4$, relaxed (see text); (d) $h_r = 3$.

FIG. 6: Angle-averaged magnetic structure factor at $T = 0$ for the random Potts field model with $h_r = \infty$ on $64 \times 64 \times 64$ simple cubic lattices, log-log plot. The points show averaged data from four samples, using four states from each sample, one from each [1,1] direction.

(a) Random state-blocking model hot start four L=64 SC samples

Legend: T=1.0, T=1.1, T=1.2, T=1.3, T=1.4, T=1.5, T=1.6, T=1.7, T=1.8, T=1.9, T=2.0, T=2.1, T=2.2, T=2.3, T=2.4

(b) hot start $h_r = 6$ four L=64 SC samples

Legend: T=1.1, T=1.2, T=1.3, T=1.4, T=1.5, T=1.6, T=1.7, T=1.8, T=1.9, T=2.0

(a)

S(k)

T=0.8
T=0.9
T=1.0
T=1.1
T=1.2
T=1.3
T=1.4

$h_r = 6$
cold [1,1] start
four L=64 SC samples

k

(b)

S(k)

T=0.8
T=0.9
T=1.0
T=1.1
T=1.2
T=1.3
T=1.4
T=1.5
T=1.6
T=1.7

$h_r = 4$
cold [1,1] start
four L=64 samples

k

(c)

S(k)

T=1.4
T=1.5
T=1.6
T=1.7

$h_r = 4$
cold [1,1] start, relaxed
four L=64 SC samples

k

(d)

S(k)

T=1.20
T=1.25
T=1.30
T=1.35

$h_r = 3$
cold [1,0] start
four L=64 samples

k

random state-blocking model
average over all [1,1] directions
for four L=64 SC samples
$E_0/J = -2.01$
$M_0 = 0.68$

T=0

S(k)

k